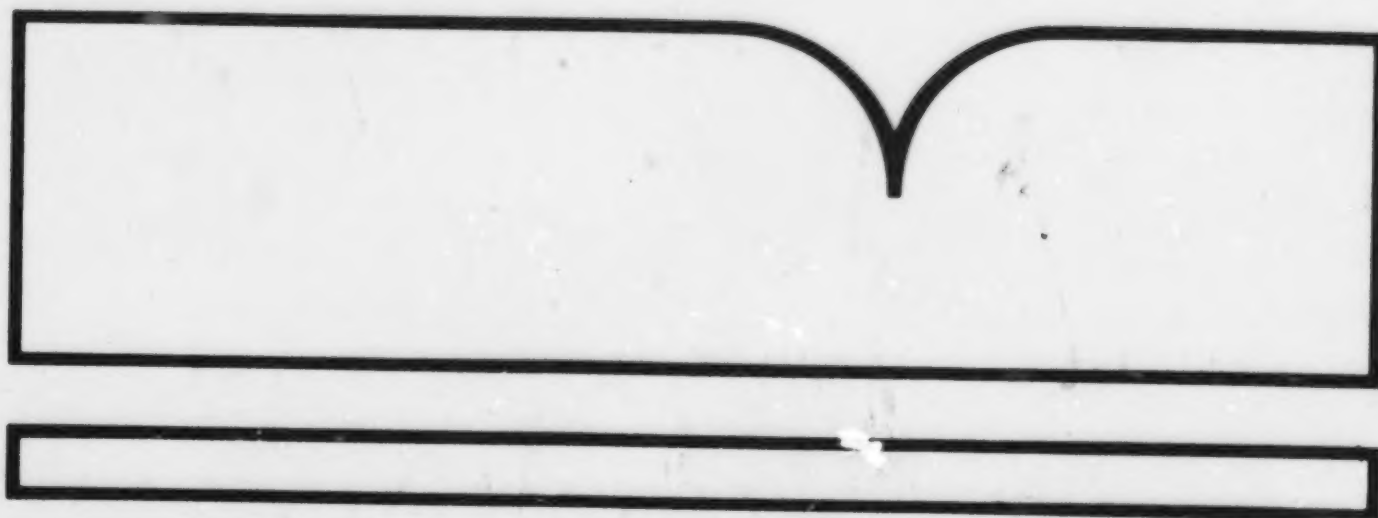


PB84-130434

Fortran Program to Re-Order
Quan Lists by Library Number

(U.S.) Municipal Environmental Research Lab.
Cincinnati, OH

1983



U.S. Department of Commerce
National Technical Information Service

NTIS

A FORTRAN PROGRAM TO RE-ORDER QUAN LISTS BY LIBRARY NUMBER

by

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Submitted to the
Users' Program Exchange Newsletter
of
Finnigan-Mat Institute

MUNICIPAL ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
CINCINNATI, OH 45268

TECHNICAL REPORT DATA (Please read Instructions on the reverse before completing)		
1. REPORT NO. EPA-600/D-84-010	2.	3. RECIPIENT'S ACCESSION NO. PB8 4 13043 4
4. TITLE AND SUBTITLE A FORTRAN PROGRAM TO RE-ORDER QUAN LISTS BY LIBRARY NUMBER	5. REPORT DATE 1983	
7. AUTHOR(S) Barry M. Austern	6. PERFORMING ORGANIZATION CODE	
9. PERFORMING ORGANIZATION NAME AND ADDRESS Municipal Environmental Research Laboratory-Cin., OH Waste Identification and Analysis Section Wastewater Research Division Cincinnati, Ohio 45268	8. PERFORMING ORGANIZATION REPORT NO.	
12. SPONSORING AGENCY NAME AND ADDRESS U.S. Environmental Protection Agency Municipal Environmental Research Laboratory-Cin., OH Wastewater Research Division Cincinnati, Ohio 45268	10. PROGRAM ELEMENT NO.	
15. SUPPLEMENTARY NOTES Contact: Barry M. Austern, (513) 684-7638	11. CONTRACT/GRANT NO.	
16. ABSTRACT If, for some reason, the quantitation list produced by a Finnigan-INCOS GC/MS data system is not in the same order as the quantitation library, then this program will reorder the list so that it is.	13. TYPE OF REPORT AND PERIOD COVERED	
	14. SPONSORING AGENCY CODE EPA/600/600/14.	
17. KEY WORDS AND DOCUMENT ANALYSIS		
a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. CCSATI Field/Group
18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES 8
	20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE

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A FORTRAN PROGRAM TO RE-ORDER QUAN LISTS BY LIBRARY NUMBER
by

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Generally, INCOS quantitation lists are written by using a reverse library search routine based on a library or library list which, of course, has a particular order. This is the order in which one is used to seeing the quantitation report and is the convenient order in which to report data.

Often, however, for some reason or another, a quantitation report can be faulty and some compounds must be requantitated. Some reasons for this may be, for example, a retention time shift out of the window or a misidentification by the software when two compounds with similar spectra and retention times, such as anthracene and phenanthrene are both of interest. In such cases the most appropriate thing to do is to perform a manual quantitation and, using EDQL, remove the offending entry from the list. This, however, puts the list out of order. If one is used to finding anthracene as the tenth entry on the list, one might now find it as the twenty-seventh.

The attached program, QUANSORT, alleviates this problem. It takes a quantitation list up to eighty entries long (the longest possible standard INCOS quanlist), sorts it in order of library entry number, and rewrites the corrected list to the disk. It is MSDS-compatible; to use it type RUN QUANSORT. Please note the following two facts: The name of the file to be sorted goes in \$1, not \$8 (although changing the equivalence statement to EQUIVALENCE (JDESC(1), IDFILE(1,4))

would probably change that) and the program sorts only on library number, not library name and all entries should, therefore, be from the same library in order not to get nonsense. (The program could, if one wishes, be rewritten to do a preliminary sort based on word #26 of the entry before sorting based on word #27, but I did not see the necessity).

PROGRAM GUANSORT SOURCE FILE

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PURPOSE: SORT A QUANLIST IN ORDER OF LIBRARY NUMBER
TO WORK OPTIMALLY, ALL ENTRIES MUST BELONG TO
SAME LIBRARY.

LOAD FILE

GL
L/F CMAIN+MFLIB+GUANSORT+
FMOPN+FMRD+FMWRT+FMCLS+IFORMAT
S/F 1: GUANSORT. MS, CDESC: . END
E

PARAMETER NUMG=80, NUMT=5, LEN=27, TTD=10, TTI=11

IG ARRAY FOR MAIN. GL

COMMON/CDATA/IG(LEN, NUMG)

NEXT COMMON FOR MAIN QUAN LIST

COMMON/CQUAN/IFILE(7), IDATE(4), IRUNTIME, FMASS, SMASS, ISCAN,
1 RET, METH(2), AREA, HIT, LNAME, LNUM

COMMON/CDESC/IDESC(13)

COMMON/CMAIN/IDUM(3), ITEMP(15), IDFILE(12, 6), ISFILE(11, 4), JDUM(24),
1 ISCN(45), IACG(100), IDATA(45)

INTEGER JDESC(13), JG(27), ; JG IS TEMP ARRAY FOR FMRD ROUTINES
1 SAMPLE(32), ICONDITIONS(32), ACCOUNT(4), IARRAY(27)

EQUIVALENCE (JDESC(1), ISFILE(1, 1)), ; DATA FILE \$1 IN STAT DISP.
1 (SAMPLE, IACG(10)),
1 (ICONDITIONS, IACG(42)),
1 (ACCOUNT, IACG(82))

READ DATA FROM QUAN LIST TO BE MODIFIED

JDESC(10)="QL"

CALL FMOPR(JDESC, JCH, \$7000, IEE)

DO 30 IC=1, NUMG ; NUMG IS 80 MAX POSSIBLE ENTRIES IN QUAN LIST

CALL FMRD(JG, JCH, LEN, \$40, IEE)

DO 31 I=1, LEN ; LEN=27 IE. NUMBER WORDS PER ENTRY

IG(I, IC)=JG(I)

CONTINUE

MAXG=IC-1 ; MAXG IS NUMBER OF ENTRIES READ

CALL FMCLS(JCH, \$7000)

DO 300 I=1, MAXG

DO 310 J=1, MAXG

IF(IG(27, I).GT.IG(27, J))GO TO 310

DO 400 K=1, 27

IARRAY(K)=IG(K, I)

CONTINUE; FIRST STEP IN PARKING PROCESS

DO 410 K=1, 27

IG(K, I)=IG(K, J)

DO 420 K=1, 27

IG(K, J)=IARRAY(K)

ARRAYS ARE NOW SWITCHED

CONTINUE

CONTINUE

CALL FMOPN(JDESC, JCH, \$7000, IEE)

CALL FMWRT(IG, JCH, LEN*MAXG, \$7000, IEE)

CALL FMCLT(JCH, \$7000)

GO TO 9000 ; EXIT TO MSDS

ERROR SECTION

WRITE(TTD, 7001)(JDESC(I), I=4, 10)

FORMAT(" ERROR ON FILE: ", 6A2, ". ", A2)

GO TO 8900

GO TO 8900

C
B900 CALL RESET ; COULD BE CHANNELS OPEN
C
C
9000 JDESC(10)=0
C
CALL LOADIT("EXEC")
C
END